

Problem with the Derivation of the Navier-Stokes Equation by Means of Zwanzig-Mori Projection Technique of Statistical Mechanics

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Abstract

The derivation of the Navier-Stokes equation starting from the Liouville equation using projection techniques yields a friction term which is nonlinear in the velocity. Using the results of multilinear mode-coupling technique for calculating equilibrium correlation functions, it is shown that the second-order part of the term is non-zero, thus leading to an incorrect formula for the equation.

Key words: statistical thermodynamics, projection operator technique, multilinear mode-coupling theory, hydrodynamic equations

1 Introduction

The derivation of hydrodynamic equations by Zwanzig-Mori projection technique is a well-established method of statistical mechanics; see, e. g., the presentations in [1], [2]. But analyzing the results further leads to a problem which is connected to the fact that the Navier-Stokes equation is of second order in the velocity. By derivation, the friction term is nonlinear in the velocity; in order to keep the equation correct it would be necessary for the second-order part of the term to vanish. But, as is shown in this paper, the derivation furnishes an expression which is generally non-zero. Since the Navier-Stokes equation is obviously a correct formula, the question arises which features of the derivation process provide these undesired details.

2 Some basic formulas

In this section some definitions and formulas are listed which are found in the textbooks of statistical mechanics. We are working with a simple fluid, i. e. we are looking at a system of N point particles with positions \mathbf{y}_i and velocities \mathbf{v}_i which collect to the phase space variable z . Indices which number the particles are denoted by j, k, \dots . The space densities of the conserved variables mass, energy and momentum, called n, e, \mathbf{p} , are collected to a matrix a :

$$a_\alpha(\mathbf{x}) = \sum_{j=1}^N \tilde{a}_{j\alpha}(z) \delta(\mathbf{x} - \mathbf{y}_j) \quad (2.1)$$

$$\tilde{a}_{j\alpha} = \left(m, \frac{m}{2} \mathbf{v}_j^2 + \frac{1}{2} \sum_{l \neq j} \varphi(|\mathbf{y}_j - \mathbf{y}_l|), m v_{ja} \right) \quad (2.2)$$

The greek index α runs over 1, 2, a where a runs from 1 to 3 so that α attains 5 scalar values in total. m is the particle mass, $\varphi(|\mathbf{y}_j - \mathbf{y}_l|)$ the intermolecular potential which I write φ_{jl} for short. The motion of the particle system is described by the variable z as a function of time t . From this, all phase space functions, especially the variables a , are functions of time described by the Liouville equation:

$$\frac{da}{dt} = \mathcal{L}a \quad (2.3)$$

$$\mathcal{L} = \frac{1}{m} \sum_{j=1}^N (\nabla_{v_j} H \cdot \nabla_{y_j} - \nabla_{y_j} H \cdot \nabla_{v_j}) \quad (2.4)$$

The Liouville Operator \mathcal{L} is presented here as a real differential operator. H is the Hamilton function:

$$H = \sum_{j=1}^N \left(\frac{1}{2} m \mathbf{v}_j^2 + \frac{1}{2} \sum_{l \neq j} \varphi_{jl} \right) \quad (2.5)$$

The formal solution of the Liouville equation reads:

$$a(t) = e^{i\mathcal{L}t} a(0) \quad (2.6)$$

The conservation property of the a is expressed by:

$$\frac{da_\alpha}{dt} = -\nabla \cdot s = -\nabla_c s_{\alpha c} \quad (2.7)$$

s are the flux densities. Paired indices are summed over. The s show a formal structure similar to the a ; cf. (2.1). The momentum flux density reads:

$$s_{ab}(\mathbf{x}) = \sum_j \left(m v_{ja} v_{jb} - \frac{1}{2} \sum_{l \neq j} \frac{d\varphi}{dr} \Big|_{|r_{jl}|} \frac{r_{jla} r_{jlb}}{|r_{jl}|} \right) \delta(\mathbf{x} - \mathbf{y}_j) \quad (2.8)$$

Here $\mathbf{r}_{jl} = \mathbf{y}_j - \mathbf{y}_l$. - The expectation of a phase space function $A(z, N)$ with respect to the probability density $f(z, N)$ is defined:

$$\langle A \rangle = tr \{ A(z, N) f(z, N) \} \quad (2.9)$$

The definition of the Operation $tr\{\}$ reads generally:

$$tr \{ A(z, N) \} = \sum_{N=1}^{\infty} \int dz A(z, N) \quad (2.10)$$

3 Hydrodynamic equations

For the projection calculations the formalism in [1] is adopted where the time dependence of the dynamic variables is considered while the expectations are defined with respect to the probability density at time $t = 0$ (Heisenberg picture). Moreover, in exponential operators where the projector \mathcal{P} and the Operator \mathcal{L} appear together in the exponent, \mathcal{L} appears 'before' (left of) \mathcal{P} . In this paper, this is called the \mathcal{L} - \mathcal{P} formulation which stems from Zwanzig (see [3] where the Schrödinger picture is used; the succession of Operators reverses if one switches to the Heisenberg picture) while Mori [4] seems to prefer the \mathcal{P} - \mathcal{L} formulation.

The result of the derivation in [1] are the formulas (8.1.13) together with (8.1.12), (8.1.7) there; in the denotation here:

$$\frac{d\langle a_\alpha \rangle}{dt} = -\nabla_c \langle s_{\alpha c} \rangle_{L,t} + D_\alpha(t) \quad (3.1)$$

The expression for the dissipative force reads:

$$D_\alpha(\mathbf{x}, t) = -\nabla_c \int_0^t dt' \int d\mathbf{x}' R_{\alpha\beta cd}(\mathbf{x}, t, \mathbf{x}', t') \nabla'_d b_\beta(\mathbf{x}', t') \quad (3.2)$$

with the kernel function:

$$R_{\alpha\beta cd}(\mathbf{x}, t, \mathbf{x}', t') = \langle [\mathcal{G}(t', t) \hat{s}_{\alpha c}(\mathbf{x}, t)] \hat{s}_{\beta d}(\mathbf{x}', t') \rangle_{L,t'} \quad (3.3)$$

$\langle \rangle_{L,t}$ denotes the expectation with respect to the probability density of the local equilibrium $f_L(t)$:

$$f_L(t) = \psi(N) \exp(\Psi(t) - a(z) * b(t)) \quad (3.4)$$

where

$$\psi(N) = \frac{1}{N!} \left(\frac{m}{h}\right)^{3N} \quad (3.5)$$

h is Planck's constant. $*$ denotes an operation which consists of a product, a summation over a greek index and a space integration; the respective variables and indices are not written down. The conjugated parameters $b_\beta(\mathbf{x}, t)$ are:

$$b = \left\{ \beta \left(\frac{m}{2} u^2 - \mu \right), \beta, -\beta \mathbf{u} \right\} \quad (3.6)$$

here $\beta = 1/(k_B T)$; k_B is Boltzmann's constant and T the temperature; these as well as the chemical potential μ and the fluid velocity \mathbf{u} are generally functions of \mathbf{x} and t . $\Psi(t)$ is a normative quantity which ensures $\text{tr}\{f_L(t)\} = 1$. In (3.3), \hat{s} denotes the reduced flux densities:

$$\hat{s}(\mathbf{x}, t) = (1 - \mathcal{P}(t))s(\mathbf{x}) \quad (3.7)$$

\mathcal{P} is the Zwanzig-Mori projection operator; for any phase space function g , it is defined:

$$\mathcal{P}g = \langle g \rangle_L + \langle g \delta a \rangle_L * \langle \delta a \delta a \rangle_L^{-1} * \delta a \quad (3.8)$$

$\delta a = a - \langle a \rangle_L$. $\langle \rangle^{-1}$ denotes the inverse matrix. Generally $\langle \rangle_L$, and therefore \mathcal{P} , depend on time. We have $R = 0$ for $\alpha = 1$ or/and $\beta = 1$, since then the reduced fluxes are zero. $\mathcal{G}(t', t)$ is a time-ordered exponential operator:

$$\mathcal{G}(t', t) = \exp_- \left\{ \int_{t'}^t dt'' \mathcal{L}(1 - \mathcal{P}(t'')) \right\} \quad (3.9)$$

We need formula (3.1) for $\alpha = 1, a$. One obtains ([1] (8.4.1), (8.3.12) und (8.4.12)):

$$\langle s_{1c} \rangle_{L,t} = \rho u_c \quad (3.10)$$

$$\langle s_{ac} \rangle_{L,t} = \rho u_a u_c + P \delta_{ac} \quad (3.11)$$

ρ is the macroscopic mass density, and P the pressure. - From here on the processes considered are restricted. The Problem mentioned in the introduction appears even under this specialization, and the necessary formulas are considerably simplified. Constant mass density/temperature processes are considered; then, the chemical potential μ is constant too. From (3.6), the term $\beta = 2$ in (3.2) is zero; thus, the sum runs over $\beta = b$ only. Finally, I confine to stationary currents, i. e. $\mathbf{u} = \text{const}(t)$. Then, expectations of single phase space functions as well as the conjugated parameters and \mathcal{P} are constant in time; \mathcal{G} reduces to a non-ordered exponential operator. Finally, the upper limit of the time integral in (3.2) may be extended to infinity. Then it is reasonable to take the time integral under the definition of the kernel function. For $\alpha = a$, one obtains, instead of (3.2), (3.3):

$$D_a(\mathbf{x}, t) = \nabla_c \int d'\mathbf{x} R_{abcd}(\mathbf{x}, \mathbf{x}') \nabla'_d u_b(\mathbf{x}') \quad (3.12)$$

$$R_{abcd}(\mathbf{x}, \mathbf{x}') = \beta \int_0^\infty dt \langle e^{\mathcal{L}(1-\mathcal{P})t} \hat{s}_{ac}(\mathbf{x}) [\hat{s}_{bd}(\mathbf{x}')] \rangle_L \quad (3.13)$$

Finally, from (3.1), together with (3.10), (3.11), one obtains for stationary constant density/temperature currents

$$\nabla \cdot \mathbf{u} = 0 \quad (3.14)$$

$$\rho u_c \nabla_c u_a = -\nabla_a P + D_a \quad (3.15)$$

with (3.12), (3.13) for D . These are the incompressibility condition and the momentum equation for stationary constant density and temperature current.

R and D are nonlinear functionals of the velocity field. From (3.12) it is obvious that in lowest order D is linear in \mathbf{u} . One obtains this order when one takes R at $\mathbf{u} = 0$. \mathbf{u} enters R exclusively via the formula for the local equilibrium (3.4). We have:

$$f_L(z, N)|_{\mathbf{u}=0} = f_0(z, N) \quad (3.16)$$

f_0 is the probability density of the thermodynamic equilibrium for prescribed mass density and temperature:

$$f_0(z, N) = \psi(N) \exp(\Psi_0 + \beta(\mu N - H(z))) \quad (3.17)$$

Ψ_0 is the norming quantity corresponding to Ψ . R at $\mathbf{u} = 0$ is called $R^{(0)}$:

$$R_{abcd}^{(0)}(\mathbf{x} - \mathbf{x}') = \beta \int_0^\infty dt \langle e^{\mathcal{L}(1-\mathcal{P}_0)t} (\hat{s}_0)_{ac}(\mathbf{x}) \rangle (\hat{s}_0)_{bd}(\mathbf{x}') \rangle_0 \quad (3.18)$$

$$(\hat{s}_0)_{ac} = (1 - \mathcal{P}_0)s_{ac} \quad (3.19)$$

$$\mathcal{P}_0 g = \langle g \rangle_0 + \langle g \delta_0 a \rangle_0 * \langle \delta_0 a \delta_0 a \rangle_0^{-1} * \delta_0 a \quad (3.20)$$

$\langle \rangle_0$ is the expectation with respect to total equilibrium, and we have $\delta_0 a = a - \langle a \rangle_0$. Since correlations in total equilibrium are transitive, $R^{(0)}$ depends on the single space variable $\mathbf{x} - \mathbf{x}'$ only. Provided the space integral over $R^{(0)}$ exists, formula (3.12), in the linear approximation, can be localized. The space integral resembles the quantity in [1], Gl. (8.5.20); though the formula is obtained there in a somewhat different way. The integral obeys several symmetries, which lead to the expression [1] (8.5.21); in the denotation used here ($D^{(1)}$ is the linear part of D):

$$D_a^{(1)}(\mathbf{x}) = \tilde{\gamma}_{abcd} \nabla_c \nabla_d u_b(\mathbf{x}) \quad (3.21)$$

$$\tilde{\gamma}_{abcd} = \int d\mathbf{x} R_{abcd}^{(0)}(\mathbf{x}) = (\delta_{ab}\delta_{cd} + \delta_{ad}\delta_{bc})\eta + \delta_{ac}\delta_{bd}(\varsigma - \frac{2}{3}\eta) \quad (3.22)$$

η, ς are the (dynamical) shear and bulk viscosity. If this is introduced into (3.21), and (3.14) is allowed for, ς eliminates, and (3.15) changes to:

$$\rho u_c \nabla_c u_a = -\nabla_a P + \eta \nabla^2 u_a \quad (3.23)$$

This is the Navier-Stokes equation für stationary constant density/temperature flow.

4 2^{nd} order term of the friction force

The Navier-Stokes equation (3.23) is of second order in the velocity. In order that it results correctly from the momentum equation (3.15) as an approximation for small Reynolds numbers, the 2^{nd} order part $D^{(2)}$ of the friction force must vanish. This part is built in (3.12) with the linear part $R^{(1)}$ of the kernel function (3.13). By Taylor's theorem, the latter reads:

$$R_{abcd}^{(1)}(\mathbf{x}, \mathbf{x}') = \int d\mathbf{x}'' \frac{\delta R_{abcd}(\mathbf{x}, \mathbf{x}')}{\delta u_e(\mathbf{x}'')} \big|_{\mathbf{u}=0} u_e(\mathbf{x}'') \quad (4.1)$$

It is useful to express the functional derivative with respect to \mathbf{u} by the derivatives with respect to the conjugated parameters b_ϵ (3.6). These are parametrically related to \mathbf{u} ; since b_1 is of 2^{nd} order in \mathbf{u} and $b_2 = \text{const}(\mathbf{u})$, for $\mathbf{u} = \mathbf{0}$ only the index value $\epsilon = e$ remains, and we have:

$$\frac{\delta R_{abcd}(\mathbf{x}, \mathbf{x}')}{\delta u_e(\mathbf{x}'')} \big|_{\mathbf{u}=\mathbf{0}} = -\beta \frac{\delta R_{abcd}(\mathbf{x}, \mathbf{x}')}{\delta b_e(\mathbf{x}'')} \big|_{\mathbf{u}=\mathbf{0}} \quad (4.2)$$

The calculation of the functional derivative is performed in the appendix. The result is (A.15):

$$\frac{\delta R_{abcd}(\mathbf{x}, \mathbf{x}')}{\delta b_e(\mathbf{x}'')} \big|_{\mathbf{u}=\mathbf{0}} = -\beta \int_0^\infty dt \langle [e^{(1-\mathcal{P}_0)\mathcal{L}t} (\hat{s}_0)_{ac}(\mathbf{x})] (\hat{s}_0)_{bd}(\mathbf{x}') p_e(\mathbf{x}'') \rangle_0 \quad (4.3)$$

With (4.1), (4.2), this yields:

$$\begin{aligned} R_{abcd}^{(1)}(\mathbf{x}, \mathbf{x}') &= -\beta \int d\mathbf{x}'' \frac{\delta R_{abcd}(\mathbf{x}, \mathbf{x}')}{\delta b_e(\mathbf{x}'')} \big|_{\mathbf{u}=\mathbf{0}} u_e(\mathbf{x}'') \\ &= \beta^2 \int d\mathbf{x}'' \left(\int_0^\infty dt \langle [e^{(1-\mathcal{P}_0)\mathcal{L}t} (\hat{s}_0)_{ac}(\mathbf{x})] (\hat{s}_0)_{bd}(\mathbf{x}') p_e(\mathbf{x}'') \rangle_0 \right) u_e(\mathbf{x}'') \end{aligned} \quad (4.4)$$

Therefore, $D^{(2)}$ reads:

$$D_a^{(2)}(\mathbf{x}, t) = \beta^2 \nabla_c \int d\mathbf{x}' \int d\mathbf{x}'' \left(\int_0^\infty dt \langle [e^{(1-\mathcal{P}_0)\mathcal{L}t} (\hat{s}_0)_{ac}(\mathbf{x})] (\hat{s}_0)_{bd}(\mathbf{x}') p_e(\mathbf{x}'') \rangle_0 \right) u_e(\mathbf{x}'') \nabla'_d u_b(\mathbf{x}') \quad (4.5)$$

4.1 Calculation of the kernel function

In this subsection, the calculation of the kernel function in (4.5) (the quantity in parentheses) is performed, using a result of multilinear mode-coupling theory. Instead of (2.1), orthonormal phase space densities are used. By replacing the energy density e by a suitable linear combination of e and n , the densities can be made orthogonal:

$$\int d\mathbf{x} \langle \delta_0 a_\alpha(\mathbf{x}) \delta_0 a_\beta^*(0) \rangle_0 = \chi_\alpha \delta_{\alpha\beta} \quad (4.6)$$

The orthonormal variables h_α read:

$$h_\alpha = \frac{\delta_0 a_\alpha}{\sqrt{\chi_\alpha}} \quad (4.7)$$

The flux densities conjugated to the h_α are called $r_{\alpha c}$, the corresponding reduced quantities $\hat{r}_{\alpha c} = (1 - \mathcal{P}_0)r_{\alpha c}$. By introducing the new definitions into (4.5) one obtains:

$$D_a^{(2)}(\mathbf{x}) = \beta^{\frac{1}{2}} \rho^{\frac{3}{2}} \nabla_c \int d\mathbf{x}' \int d\mathbf{x}'' \left(\int_0^\infty dt \langle [e^{(1-\mathcal{P}_0)\mathcal{L}t} \hat{r}_{ac}(\mathbf{x})] \hat{r}_{bd}(\mathbf{x}') p_e(\mathbf{x}'') \rangle_0 \right) u_e(\mathbf{x}'') \nabla'_d u_b(\mathbf{x}') \quad (4.8)$$

The calculation is done in Fourier space. We have:

$$D_a^{(2)}(\mathbf{k}) = \beta^{\frac{1}{2}} \rho^{\frac{3}{2}} \frac{1}{(2\pi)^6} \int d\mathbf{q} N_{abc}(\mathbf{k}, \mathbf{q}, \mathbf{k} - \mathbf{q}) u_b(\mathbf{q}) u_c(\mathbf{k} - \mathbf{q}) \quad (4.9)$$

$$N_{abc}(\mathbf{k}, \mathbf{q}, \mathbf{q}') = k_d q_e \int_0^\infty dt \langle [e^{(1-\mathcal{P}_0)\mathcal{L}t} \hat{r}_{ad}(\mathbf{k})] \hat{r}_{be}^*(\mathbf{q}) h_c^*(\mathbf{q}') \rangle_0 \quad (4.10)$$

The kernel function N is to be calculated. The multilinear mode-coupling technique is for calculating correlation functions which are defined with the original exponential operator $\exp\{\mathcal{L}t\}$, that is, without $1 - \mathcal{P}_0$. In order to find a connection, one uses the operator identity:

$$e^{(1-\mathcal{P}_0)\mathcal{L}t} = e^{\mathcal{L}t} - \int_0^t dt' e^{\mathcal{L}t'} \mathcal{P} \mathcal{L} e^{(1-\mathcal{P}_0)\mathcal{L}(t-t')} \quad (4.11)$$

Application results in the formula:

$$N_{abc}(\mathbf{k}, \mathbf{q}, \mathbf{q}') = i q_e \int_0^\infty dt \left\{ \int_0^t dt' \tilde{\Gamma}_{\alpha\epsilon}(\mathbf{k}, t - t') \langle [e^{\mathcal{L}t'} h_\epsilon(\mathbf{k})] \hat{r}_{be}^*(\mathbf{q}) h_c^*(\mathbf{q}') \rangle - i k_d \langle [e^{\mathcal{L}t} \hat{r}_{ad}(\mathbf{k})] \hat{r}_{be}^*(\mathbf{q}) h_c^*(\mathbf{q}') \rangle \right\} \quad (4.12)$$

$$\tilde{\Gamma}_{\alpha\beta}(\mathbf{k}, t) = k_c k_d \langle \tilde{\Phi}_{\alpha c}(t) \tilde{\Phi}_{\beta d}^*(t) \rangle(\mathbf{k})|_{\mathbf{k}=0} \quad (4.13)$$

$$\tilde{\Phi}_{\alpha c}(\mathbf{k}, t) = e^{(1-\mathcal{P}_0)\mathcal{L}t} \hat{r}_{\alpha c}(\mathbf{k}) \quad (4.14)$$

$\langle A B^* \rangle(\mathbf{k})$ is defined to be the Fourier transform of the correlation $\langle A(\mathbf{x}) B(0) \rangle$. $\tilde{\Gamma}_{\alpha\beta}$ is the localized memory function of the process. The \sim points to the fact that the function $\tilde{\Phi}$ is defined with the aid of the projection operator \mathcal{P}_0 which is linear in the microscopic densities h_α (see below for the discussion of the projection operator of the multilinear technique). It is assumed that the time integral of the memory function exists:

$$\tilde{\gamma}_{\alpha\beta}(\mathbf{k}) = \int_0^\infty dt \tilde{\Gamma}_{\alpha\beta}(\mathbf{k}, t) \quad (4.15)$$

Then, $\tilde{\Gamma}$ in (4.12) can be "localized" in time. $\tilde{\gamma}_{\alpha\beta}$ is found to be diagonal; thus, if $\alpha = a$, then $\beta = b$. The other correlations appearing in (4.12) can be related to the triple correlation C_3 of the orthonormal densities:

$$(C_3)_{\alpha\beta\gamma}(t) = \langle [e^{\mathcal{L}t} h_\alpha] h_\beta^* h_\gamma^* \rangle \quad (4.16)$$

Finally, for the application in (4.9) it is possible to replace N_{abc} by the symmetrized form $\frac{1}{2}(N_{abc} + N_{acb})$ which is denoted by the same symbol. One obtains from (4.12):

$$\begin{aligned} 2N_{abc} = & -\tilde{\kappa}_{a\epsilon} \left[(C_3)_{\epsilon bc}(0) - \int_0^\infty dt (i\omega_{b\tau}(C_3)_{\epsilon\tau c}(t) + i\omega_{c\tau}(C_3)_{\epsilon b\tau}(t)) \right] \\ & - \frac{\partial(C_3)_{abc}(t)}{\partial t} \Big|_{t=0} - i\omega_{b\tau}(C_3)_{a\tau c}(0) - i\omega_{c\tau}(C_3)_{ab\tau}(0) \end{aligned} \quad (4.17)$$

$$\tilde{\kappa}_{\alpha\beta} = \tilde{\gamma}_{\alpha\beta} + i\omega_{\alpha\beta} \quad (4.18)$$

$$\omega_{\alpha\beta}(\mathbf{k}) = k_d \langle r_{\alpha d} h_\beta^* \rangle(\mathbf{k})|_{\mathbf{k}=0} \quad (4.19)$$

N and C_3 depend on three wave numbers $\mathbf{k}, \mathbf{q}, \mathbf{q}'$. The wave numbers of the other quantities in (4.17) are $\tilde{\gamma}_{a\epsilon}(\mathbf{k}), \omega_{a\epsilon}(\mathbf{k}), \omega_{b\tau}(\mathbf{q}), \omega_{c\tau}(\mathbf{q}')$.

By (4.17), we connected the kernel function N to the triple correlation C_3 which is defined with the exponential Operator $\exp\{Lt\}$. The formula for the latter we take from the multilinear mode coupling theory for correlation functions [6]. This theory is worked out in Fourier space *before* performing the thermodynamic limit. Then, the correlations are proportional to the Volume V . In what follows all correlations are divided by V ; then, V does not appear any more in the formulas. From the formulas (31), (30) there, one obtains, with the denotation used here:

$$(C_3)_{\alpha\beta\gamma}(t) = (C_2)_{\alpha\epsilon}(t) J_{\epsilon\beta\gamma} - \int_0^t dt' (C_2)_{\alpha\epsilon}(t-t') i k_d S_{\epsilon\rho\tau d} (C_2)_{\rho\beta}(t') (C_2)_{\tau\gamma}(t') \quad (4.20)$$

$$(C_2)_{\alpha\beta}(t) = \langle [e^{\mathcal{L}t} h_\alpha] h_\beta^* \rangle \quad (4.21)$$

$$S_{\alpha\beta\gamma d} = \langle r_{\alpha d} h_\beta^* h_\gamma^* \rangle|_{\mathbf{q}, \mathbf{k}, \mathbf{k}'=0} \quad (4.22)$$

$$J_{\alpha\beta\gamma} = (C_3)_{\alpha\beta\gamma}(0)|_{\mathbf{q}, \mathbf{k}, \mathbf{k}'=0} \quad (4.23)$$

For C_2 , one obtains, after "localization" in time corresponding to (4.15):

$$(\dot{C}_2)_{\alpha\beta}(t) = -\kappa_{\alpha\gamma} (C_2)_{\gamma\beta}(t) \quad (4.24)$$

$$\kappa_{\alpha\beta} = \gamma_{\alpha\beta} + i\omega_{\alpha\beta} \quad (4.25)$$

γ is the dissipation matrix defined corresponding to (4.15) but with the projection operator of the multilinear Theory which is nonlinear in the h_α . When one introduces (4.20) into (4.17), one obtains an expression for N which contains the matrices $\omega, \gamma, \tilde{\gamma}, J$ and S . For the present intention to check whether the 2^{nd} order part of the friction force is different from zero, one can neglect the difference between γ and $\tilde{\gamma}$. Then one finds:

$$N_{abc} = \frac{1}{2} (\gamma_{b\rho} \delta_{c\sigma} + \delta_{b\rho} \gamma_{c\sigma}) (\kappa_{\rho\epsilon} \delta_{\sigma\tau} + \delta_{\rho\epsilon} \kappa_{\sigma\tau})^{-1} i k_d S_{a\epsilon\tau d} \quad (4.26)$$

The kernel function N will be used to calculate the friction force term D_2 (4.9), with the incompressibility condition (3.14) $\mathbf{k} \cdot \mathbf{u} = 0$ to be incorporated. This being accounted for, for N there remains a relevant part:

$$N_{abc} = \frac{1}{2} i k_d S_{abcd} \quad (4.27)$$

One finds:

$$S_{abcd} = \frac{1}{\sqrt{\rho\beta}} (\delta_{ab} \delta_{cd} + \delta_{ac} \delta_{bd} - \lambda \delta_{ad} \delta_{bc}) \quad (4.28)$$

$$\lambda = \frac{\partial P}{\partial \beta} \Big|_{\rho} \left(\frac{\partial \epsilon}{\partial \beta} \Big|_{\rho} \right)^{-1} \quad (4.29)$$

and by introduction into (4.9):

$$D_a^{(2)}(\mathbf{k}) = \frac{\rho}{(2\pi)^6} \int d\mathbf{q} \left(ik_d u_a(\mathbf{q}) u_d(\mathbf{k} - \mathbf{q}) - \frac{\lambda}{2} ik_a u_b(\mathbf{q}) u_b(\mathbf{k} - \mathbf{q}) \right) \quad (4.30)$$

It is seen that the 2^{nd} order part of the friction force is calculated to be not zero. The formula will be evaluated in the next section.

5 Consequences

The consequences of the result (4.30) will show up clearly if one uses the solenoidal form of the Navier-Stokes equation, that is, the equation with the pressure term eliminated. Instead of (3.23), the stationary form of the equation is chosen, and the 2^{nd} order term of the friction force $D^{(2)}_a = \nabla_c R_{ac}^{(2)}$ is added. Here R_{ac} with two indices is the stress tensor which should not be confounded with the kernel function R_{abcd} . The calculation is performed in Fourier space. The Navier-Stokes equation supplemented by $D^{(2)}$ reads:

$$\rho \left(\frac{\partial u_a}{\partial t} + \nu k^2 u_a \right) = -ik_a P - ik_c \left(\frac{\rho}{(2\pi)^3} \int d\mathbf{q} u_a(\mathbf{q}) u_c(\mathbf{k} - \mathbf{q}) - R_{ac}^{(2)} \right) \quad (5.1)$$

After a short calculation (see, e. g., [5] appendix D, (D34)) the solenoidal form of the equation is obtained:

$$\rho \left(\frac{\partial u_a}{\partial t} + \nu k^2 u_a \right) = -ik_c \varepsilon_{ab} \left(\frac{\rho}{(2\pi)^3} \int d\mathbf{q} u_b(\mathbf{q}) u_c(\mathbf{k} - \mathbf{q}) - R_{bc}^{(2)} \right) \quad (5.2)$$

$$\varepsilon_{ab} = \delta_{ab} - \hat{k}_a \hat{k}_b \quad (5.3)$$

$\hat{\mathbf{k}}$ is the unit vector attached to \mathbf{k} . Now, for D_2 the result (4.30) is introduced. Since we have $k_c \varepsilon_{ac} = 0$, the 2^{nd} term does not contribute. One obtains:

$$ik_c \varepsilon_{ab} \left(\frac{\rho}{(2\pi)^3} \int d\mathbf{q} u_b(\mathbf{q}) u_c(\mathbf{k} - \mathbf{q}) - R_{bc}^{(2)} \right) = 0 \quad (5.4)$$

The 2^{nd} order part of the friction force cancels the convolution term of the Navier-Stokes equation, so that the equation reduces to its linear part. Since by phenomenological evidence the convolution term is an essential part of the equation, this theoretical result cannot be correct.

6 Summary

The derivation of hydrodynamic equations by Zwanzig-Mori projection technique has been reviewed. For simplicity, incompressible constant density/temperature fluids have been considered. The friction force term in the momentum equation is a nonlinear functional of the fluid velocity; when the linear approximation is taken, the Navier-Stokes equation is obtained. In the present paper, the second-order term of the friction force has been calculated. It contains a three-point time correlation function which has been evaluated using a result of multilinear mode-coupling theory; the final result is (4.30). Since the Navier-Stokes equation is second order in the velocity, in order to obtain it properly as an approximation of the momentum equation for small Reynolds numbers, one would expect the second-order part of the friction force to vanish. Thus, (4.30) is clearly an undesired result; it would be very valuable to know which detail of the derivation may be responsible for it.

A Appendix: Calculation of the functional derivative

In order to calculate the derivative in (4.2), the formula for R (3.13) is written in detail:

$$R_{abcd}(\mathbf{x}, \mathbf{x}') = \beta \int_0^\infty dt \operatorname{tr} \{ f_L [e^{\mathcal{L}(1-\mathcal{P})t} (1-\mathcal{P}) s_{ac}(\mathbf{x})] (1-\mathcal{P}) s_{bd}(\mathbf{x}') \} \quad (A.1)$$

The expression depends on b_e 4-fold, namely, in the formula for the local equilibrium f_L , and in \mathcal{P} appearing 3-fold. For abbreviation, the formula is written:

$$\frac{\delta R_{abcd}(\mathbf{x}, \mathbf{x}')}{\delta b_e(\mathbf{x}'')} = \sum_{i=1}^4 \left[\frac{\delta R}{\delta b} \right]^{(i)} \quad (A.2)$$

In the consecutive formulas, in the first row the definition of the several parts is expressed. For the calculation some auxiliary theorems for projection operators are used, which can be found in the text books. For the 1st partial term:

$$\begin{aligned} \left[\frac{\delta R_{abcd}}{\delta b_e(\mathbf{x}'')} \right]^{(1)} &= \beta \int_0^\infty dt \operatorname{tr} \left\{ \frac{\delta f_L}{\delta b_e(\mathbf{x}'')} [e^{\mathcal{L}(1-\mathcal{P})t} \hat{s}_{ac}(\mathbf{x})] \hat{s}_{bd}(\mathbf{x}') \right\} \\ &= -\beta \int_0^\infty dt \langle [e^{\mathcal{L}(1-\mathcal{P})t} \hat{s}_{ac}(\mathbf{x})] \hat{s}_{bd}(\mathbf{x}') \delta p_e(\mathbf{x}'') \rangle_L \end{aligned} \quad (\text{A.3})$$

The 2nd term:

$$\begin{aligned} \left[\frac{\delta R_{abcd}}{\delta b_e(\mathbf{x}'')} \right]^{(2)} &= -\beta \int_0^\infty dt \langle [e^{\mathcal{L}(1-\mathcal{P})t} \hat{s}_{ac}(\mathbf{x})] \frac{\delta \mathcal{P}}{\delta b_e(\mathbf{x}'')} s_{bd}(\mathbf{x}') \rangle_L \\ &= \beta \int_0^\infty dt \langle [e^{\mathcal{L}(1-\mathcal{P})t} \hat{s}_{ac}(\mathbf{x})] \mathcal{P} \hat{s}_{bd}(\mathbf{x}') \delta p_e(\mathbf{x}'') \rangle_L \end{aligned} \quad (\text{A.4})$$

The Operator \mathcal{P} acts on everything on the right (provided the action is not limited by parentheses). The 3rd term:

$$\begin{aligned} \left[\frac{\delta R_{abcd}}{\delta b_e(\mathbf{x}'')} \right]^{(3)} &= -\beta \int_0^\infty dt \langle [e^{\mathcal{L}(1-\mathcal{P})t} \frac{\delta \mathcal{P}}{\delta b_e(\mathbf{x}'')} s_{ac}(\mathbf{x})] \hat{s}_{bd}(\mathbf{x}') \rangle_L \\ &= \beta \int_0^\infty dt \langle [e^{\mathcal{L}(1-\mathcal{P})t} \mathcal{P} \hat{s}_{ac}(\mathbf{x}) \delta p_e(\mathbf{x}'')] \hat{s}_{bd}(\mathbf{x}') \rangle_L \\ &= \beta \int_0^\infty dt \langle [e^{(1-\mathcal{P})\mathcal{L}t} (1-\mathcal{P}) \mathcal{P} \hat{s}_{ac}(\mathbf{x}) \delta p_e(\mathbf{x}'')] \hat{s}_{bd}(\mathbf{x}') \rangle_L = 0 \end{aligned} \quad (\text{A.5})$$

The 4th term is defined:

$$\left[\frac{\delta R_{abcd}}{\delta b_e(\mathbf{x}'')} \right]^{(4)} = \beta \int_0^\infty dt \langle [\frac{\delta e^{\mathcal{L}(1-\mathcal{P})t}}{\delta b_e(\mathbf{x}'')} \hat{s}_{ac}(\mathbf{x})] \hat{s}_{bd}(\mathbf{x}') \rangle_L \quad (\text{A.6})$$

The formula for the derivative of the exponential operator reads:

$$\frac{\delta e^{\mathcal{L}(1-\mathcal{P})t}}{\delta b_e(\mathbf{x}'')} = \int_0^t dt' e^{\mathcal{L}(1-\mathcal{P})t'} \mathcal{L} \mathcal{P} \delta p_e(\mathbf{x}'') (1-\mathcal{P}) e^{\mathcal{L}(1-\mathcal{P})(t-t')} \quad (\text{A.7})$$

We use the identity:

$$\int_0^\infty dt \int_0^t dt' A(t', t-t') = \int_0^\infty dt \int_0^\infty dt' A(t', t) \quad (\text{A.8})$$

One obtains:

$$\begin{aligned} \left[\frac{\delta R_{abcd}}{\delta b_e(\mathbf{x}'')} \right]^{(4)} &= \beta \int_0^\infty dt \int_0^\infty dt' \langle [e^{\mathcal{L}(1-\mathcal{P})t'} \mathcal{L} \mathcal{P} \delta p_e(\mathbf{x}'') (1-\mathcal{P}) e^{\mathcal{L}(1-\mathcal{P})t} \hat{s}_{ac}(\mathbf{x})] \hat{s}_{bd}(\mathbf{x}') \rangle_L \\ &= \beta \int_0^\infty dt \int_0^\infty dt' \langle [e^{(1-\mathcal{P})\mathcal{L}t'} (1-\mathcal{P}) \mathcal{L} \mathcal{P} \delta p_e(\mathbf{x}'') e^{(1-\mathcal{P})\mathcal{L}t} \hat{s}_{ac}(\mathbf{x})] \hat{s}_{bd}(\mathbf{x}') \rangle_L \\ &= \beta \int_0^\infty dt \int_0^\infty dt' \langle [\frac{d}{dt'} e^{(1-\mathcal{P})\mathcal{L}t'} \mathcal{P} \delta p_e(\mathbf{x}'') e^{(1-\mathcal{P})\mathcal{L}t} \hat{s}_{ac}(\mathbf{x})] \hat{s}_{bd}(\mathbf{x}') \rangle_L \end{aligned} \quad (\text{A.9})$$

The integration over t' is performed:

$$\begin{aligned} \left[\frac{\delta R_{abcd}}{\delta b_e(\mathbf{x}'')} \right]^{(4)} &= \beta \int_0^\infty dt \left\{ \lim_{t' \rightarrow \infty} \langle [e^{(1-\mathcal{P})\mathcal{L}t'} \mathcal{P} \delta p_e(\mathbf{x}'') e^{(1-\mathcal{P})\mathcal{L}t} \hat{s}_{ac}(\mathbf{x})] \hat{s}_{bd}(\mathbf{x}') \rangle_L \right. \\ &\quad \left. - \langle [\mathcal{P} \delta p_e(\mathbf{x}'') e^{(1-\mathcal{P})\mathcal{L}t} \hat{s}_{ac}(\mathbf{x})] \hat{s}_{bd}(\mathbf{x}') \rangle_L \right\} \end{aligned} \quad (\text{A.10})$$

In the 1st term, the operation \mathcal{P} is performed by (3.8):

$$\begin{aligned}
& \beta \int_0^\infty dt \lim_{t' \rightarrow \infty} \langle [e^{(1-\mathcal{P})\mathcal{L}t'} \mathcal{P} \delta p_e(\mathbf{x}'') e^{(1-\mathcal{P})\mathcal{L}t} \hat{s}_{ac}(\mathbf{x})] \hat{s}_{bd}(\mathbf{x}') \rangle_L \\
&= \beta \int_0^\infty dt \lim_{t' \rightarrow \infty} \langle [e^{(1-\mathcal{P})\mathcal{L}t'} \left\{ \langle \delta p_e(\mathbf{x}'') e^{(1-\mathcal{P})\mathcal{L}t} \hat{s}_{ac}(\mathbf{x}) \rangle_L \right. \\
&\quad \left. + \langle \delta p_e(\mathbf{x}'') [e^{(1-\mathcal{P})\mathcal{L}t} \hat{s}_{ac}(\mathbf{x})] \delta a \rangle_L \langle \delta a \delta a \rangle_L^{-1} \delta a \right\} \hat{s}_{bd}(\mathbf{x}') \rangle_L \\
&= \beta \int_0^\infty dt \left\{ \langle \delta p_e(\mathbf{x}'') e^{(1-\mathcal{P})\mathcal{L}t} \hat{s}_{ac}(\mathbf{x}) \rangle_L \langle \hat{s}_{bd}(\mathbf{x}') \rangle_L \right. \\
&\quad \left. + \langle \delta p_e(\mathbf{x}'') [e^{(1-\mathcal{P})\mathcal{L}t} \hat{s}_{ac}(\mathbf{x})] \delta a \rangle_L \langle \delta a \delta a \rangle_L^{-1} \lim_{t' \rightarrow \infty} \langle [e^{(1-\mathcal{P})\mathcal{L}t'} \delta a] \hat{s}_{bd}(\mathbf{x}') \rangle_L \right\} \quad (\text{A.11})
\end{aligned}$$

Here, the 2nd factor of the 1st term vanishes, therefore the 1st term vanishes in total. All expressions are finely to be taken at $b = b_0$. Therefore, the limit $\lim_{t' \rightarrow \infty}$ of a correlation function in thermodynamic equilibrium must be performed. One assumes that this equates to the product of the expectations of the factor functions. This assumption has been checked with the aid of the multilinear mode coupling theory, and verified for the special cases appearing here:

$$\lim_{t' \rightarrow \infty} \langle [e^{(1-\mathcal{P}_0)\mathcal{L}t'} \delta_0 a] (1 - \mathcal{P}_0) s_{bd}(\mathbf{x}') \rangle_0 = \langle \delta_0 a \rangle_0 \langle (1 - \mathcal{P}_0) s_{bd}(\mathbf{x}') \rangle_0 = 0 \quad (\text{A.12})$$

with \mathcal{P}_0 by (3.20). Therefore, the 2nd term in (A.11) is zero also, so this is true for the 1st term in (A.10) in total. Finally, the 2nd term in (A.10) vanishes, since one factor starts with \mathcal{P} , the other with $1 - \mathcal{P}$. One obtains:

$$\left[\frac{\delta R_{abcd}}{\delta b_e(\mathbf{x}'')} \right]^{(4)} \Big|_{\mathbf{u}=0} = 0 \quad (\text{A.13})$$

Thus, we finally find that the derivative (A.2), after letting $\mathbf{u} = 0$, will be equal to the sum of the first two terms of the r. h. s.; with (A.3), (A.4):

$$\begin{aligned}
& \left[\frac{\delta R_{abcd}}{\delta b_e(\mathbf{x}'')} \right]^{(1)} + \left[\frac{\delta R_{abcd}}{\delta b_e(\mathbf{x}'')} \right]^{(2)} \\
&= -\beta \int_0^\infty dt \langle [e^{\mathcal{L}(1-\mathcal{P})t} \hat{s}_{ac}(\mathbf{x})] (1 - \mathcal{P}) \hat{s}_{bd}(\mathbf{x}') \delta p_e(\mathbf{x}'') \rangle_L \\
&= -\beta \int_0^\infty dt \langle [e^{(1-\mathcal{P})\mathcal{L}t} \hat{s}_{ac}(\mathbf{x})] \hat{s}_{bd}(\mathbf{x}') \delta p_e(\mathbf{x}'') \rangle_L \quad (\text{A.14})
\end{aligned}$$

One sees that the shortest expression results with the \mathcal{P} -before- \mathcal{L} formulation. Finally, by taking $\mathbf{u} = 0$:

$$\frac{\delta R_{abcd}(\mathbf{x}, \mathbf{x}')}{\delta b_e(\mathbf{x}'')} \Big|_{\mathbf{u}=0} = -\beta \int_0^\infty dt \langle [e^{(1-\mathcal{P}_0)\mathcal{L}t} (\hat{s}_0)_{ac}(\mathbf{x})] (\hat{s}_0)_{bd}(\mathbf{x}') p_e(\mathbf{x}'') \rangle_0 \quad (\text{A.15})$$

The last factor p_e does not show a δ any more since $\langle p_e \rangle_0 = 0$. - The calculation of the derivative has been performed in \mathcal{P} -before- \mathcal{L} formulation also. The in-between steps look somewhat different; for instance, we have $\square^{(4)} \neq 0$. The final result coincides with (A.14).

References

- [1] H. Grabert: Projection operator techniques in nonequilibrium statistical mechanics. Springer, Berlin, Heidelberg, New York (1982)
- [2] D. Zubarev, V. Morozov, G. Röpke: Statistical mechanics of nonequilibrium processes. Akademie Verlag, Berlin (1996)
- [3] R. Zwanzig, J Chem. Phys. 33: 1338 (1960)
- [4] H. Mori, Progr. Theor. Phys. 33: 423 (1965)
- [5] W. D. McComb, The Physics of Fluid Turbulence, Clarendon Press, Oxford, Reprint 1994
- [6] R. van Zon, J. Schofield, Phys. Rev. E 65 (2001), 011106